Phase Diagrams of Alcohols and Cholinium-Derived Bistriflamide Ionic Liquid Mixtures

Anabela J. L. Costa and Mário R. C. Soromenho
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal

Karina Shimizu and José N. Canongia Lopes [S]
Instituto Superior Técnico, Universidade Técnica de Lisboa, Centro de Química Estrutural, Lisboa, Portugal

Isabel M. Marrucho, José M. S. S. Esperança [C] and Luís Paulo N. Rebelo
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal
jmesp@itqb.unl.pt

Choline is an essential micronutrient, usually grouped as a B-complex vitamin, which is important in several body functions. Ionic liquids based on the cholinium cation (trimethyl-hydroxyethylammonium) have been investigated as possible environmentally friendly alternatives to conventional ionic liquids. A new family of ionic liquids inspired on the cholinium cation, alkyl-dimethyl-hydroxyethylammonium, with the alkyl chain ranging from C_2 to $C_{8,}$ combined with the bistrisflamide anion was synthesized and characterized. In this work, we have measured the temperature-composition phase diagrams of alkyl-dimethyl-hydroxyethylammonium bistriflamide ionic liquids ($1<c_n<8$) with alcohols (alkyl chains from C_4 to C_8). The coexistence curves corresponding to liquid-liquid equilibria (LLE) boundaries were visually determined and the experimental results have been correlated using a set of empirical equations capable of describing the corresponding upper critical solution temperatures loci. The different types of LLE behavior were discussed in terms of the alkyl chain length of the cation and the alkyl-chain length, branching of the solute and position of the alcohol group. Auxiliary simulation data (obtained by ab initio or by molecular dynamics methods) were used to corroborate some of the experimental findings.